Benchmark Calculations with COMSOL of the Transport of Radionuclides through Clay and Bentonite Barriers in a Geological Repository

Manuel Lorenzo Sentís*[1], Felix Altorfer[1], Martin Herfort[1], Andreas Jakob[2], Georg Kosakowski[2], Sven Friedel[3]
[1]Swiss Federal Nuclear Safety Inspectorate (ENSI)
[2]Paul Scherrer Institute (PSI)
[3]COMSOL Multiphysics GmbH
*Corresponding author: ENSI, Disposal and Safety Analyses Section (TISA), CH-5232 Villigen-ENSI, Switzerland, manuel.sentis@ensi.ch

Introduction

The sectoral plan for the selection of geological repositories for nuclear waste (spent fuel, vitrified high level and long-lived intermediate-level waste as well as for low-level waste) in Switzerland started in 2008 and will last about ten years. The Swiss Federal Nuclear Safety Inspectorate (ENSI) examines and evaluates the proposals put forward by the implementer Nagra from the point of view of safety. In order to perform independent safety analysis calculations and thus to review the safety assessments of the implementer Nagra, ENSI decided to use the program COMSOL in particular the “Earth Science Module”.

A benchmark study was carried out in collaboration with the Laboratory for Waste Management (LES) of the Paul Scherrer Institute (PSI) in order to evaluate the capabilities of the program. In this study results of four different codes were compared: PICNIC, FRAC3DVS, COMSOL (Version 3.4) and Tough2-EOS9nT. PICNIC calculations were published by Nagra for a conceptual model of a geological repository within a feasibility study (project “Opalinus Clay”). The results were reproduced by PSI with help of FRAC3DVS and an independently developed COMSOL model as well as by ENSI with COMSOL and Tough2-EOS9nT. In the feasibility study a potential site located in the geological formation Opalinus Clay in northern Switzerland was selected. To estimate the release of radionuclides to the biosphere, the complex system of caverns and tunnels was simplified into a one-dimensional (PICNIC) or into a two-dimensional (COMSOL, FRAC3DVS, Tough2-EOS9nT) conceptual model as shown in the next figure.

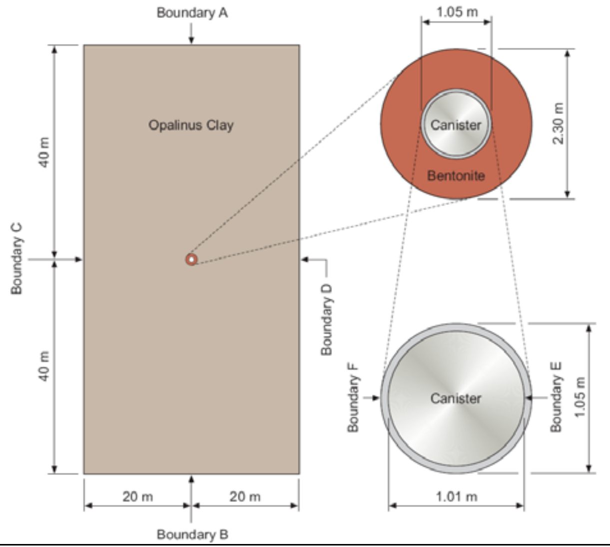

Figure 1: Conceptual Model for the calculations

Use of COMSOL Multiphysics

To study the transport of different nuclides through the different barriers of the geological repository the program COMSOL Multiphysics in particular the “Earth Science Module” was used. The study concentrated on some critical radionuclides that show only small retention in the different barriers of the geological repository: I-129, Ca-41, Cl-36, Se-79 and C-14.

The Model is based on the following three equations:

- Mass conservation of the water:

$$\frac{\partial(\phi s_f \rho_f)}{\partial t} + \nabla(\phi s_f \rho_f \vec{v}) = Q_f \tag{1}$$

with ρ_f [kg m^{-3}] for the density of water, $\vec{v}$ [m/s] the average velocity of the flow, s_f [-] the saturation of the medium, ϕ [-] the porosity of the medium and Q_f [kg m^{-3}s^{-1}] a source term for the flow of water. This equation is simplified with the elimination of the time derivative (stationary flow) and of the source term for water (weak advective flow). Furthermore the medium considered in this report is fully saturated and that means:

$$s_f = 1 \tag{2}$$

- Darcy’s law for the mass flux of water:

$$\vec{j} = \rho_f \phi \vec{v} = -\rho_f K \phi \nabla \varphi \tag{3}$$

where K [m/s] is the hydraulic conductivity and φ [m] the hydraulic potential.

Taking into account the equations (2) and (3) and the considerations at the end of the first point, the equation (1) becomes:

$$-\rho_f K \phi \Delta \varphi = 0 \tag{4}$$

- Mass conservation of the nuclides or transport equation:

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_t c_s) + \nabla \cdot [-\phi s_f \overline{\overline{D}} \nabla c + \phi s_f \vec{v} c] = \sum R_f + \sum R_s + Q \tag{5}$$

where ρ_t [kg m^{-3}] is he bulk density, c [kg m^{-3}] the concentration of the nuclide in the liquid phase and c_s [-] (the dimensions are mass of adsorbed contaminant per dry unit weight of solid) the concentration of the nuclide in the solid phase, $\overline{\overline{D}}$ [m^2/s] the hydrodynamic dispersion tensor, R_f [kg m^{-3} s^{-1}] and R_s [kg m^{-3} s^{-1}] are the terms for the reactions (sum over the different reactions for example chemical reactions, radioactive decay) of the nuclides in water and in the solid phase. For the calculations shown in this document only radioactive decay was considered and the two terms reduce to:

$$\sum R_f = \lambda c \tag{6}$$

$$\sum R_f = \lambda c_s \tag{7}$$

where λ [m^{-1}] is the decay constant of the considered nuclide. For the calculations shown in this document c_s is related to c through a linear isotherm with a sorption coefficient K_d [m^3 /kg]:

$$c_s = K_d\, c \tag{8}$$

The last term Q [kg m^{-3}s^{-1}] in equation (7) represents the solute added per unit volume of soil and per unit time.

The hydraulic boundary conditions are fixed potentials of 0 m at the top and 80 m at the bottom (boundaries A and B in Figure 1), that corresponds to a hydraulic gradient of 1 m/m (φ has units m and therefore $\nabla\varphi$ has units m/m). On the left and right part of the boundary (boundaries C and D in Figure 1) as well as on the boundary E a no-flow boundary for both, flow and transport was defined. As consequence of the corrosion of the waste container the nuclides are released from the boundary F. These release rate values originally in a tabular format are implemented into COMSOL by means of an interpolation function. As initial condition for the hydraulic potential a linear variation from the bottom to the top of the domain was set (upward flow). The initial pressure in the bentonite filling is 0.14x10^6 Pa.

The flow and the transport model are symmetric with respect to a vertical line passing through the centre of the canister and therefore only the right part was considered in the calculations. This reduces the time needed for the solution.

A two-step approach with different COMSOL models was used to solve the above-mentioned equations. In a first step the stationary equation (4) (Darcy's law model) for the water flow equation is solved and the velocity obtained is used as input for the second step, in which the transport equation (5) is solved (solute transport model). Integration coupling variables were defined on the top and bottom part of the domain in order to integrate the flow of each nuclide over these boundaries.

Results

The result of the release rates for the nuclides I-129 and Cl-36 are shown in the Figures 2 and 3. The results of COMSOL are represented in red and they are always between the results of the other codes.

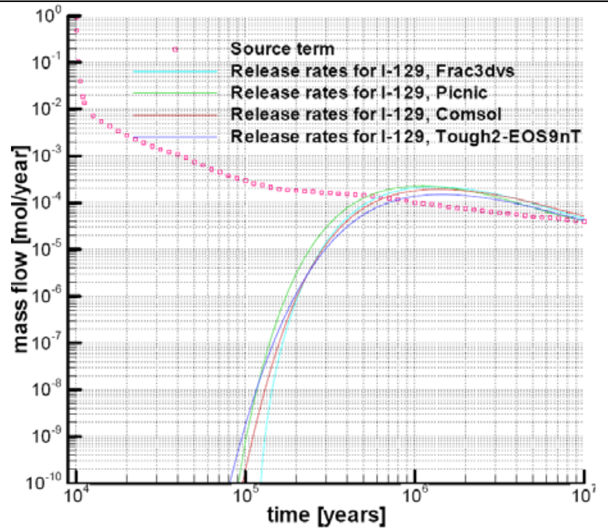

Figure 2. Release rates for I-129

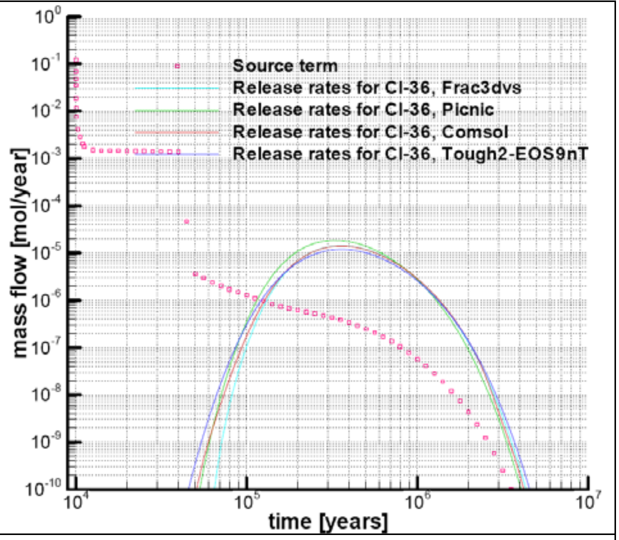

Figure 3. Release rates for Cl-36

Conclusion

The time-dependent radionuclide flux over the upper and lower boundaries for a time span of 10 million years are similar for the four different codes. Differences in the conceptualization and in the numerical methods used in the considered codes explain the slight discrepancy in the results of the calculations with the different codes. Based on these results ENSI decided to continue using COMSOL for the evaluation of the proposal sites by Nagra within the sectoral plan.